REMARKS

The Applicants have herein amended Claims 1, 18, 20, 22, 23, and 35. Claims 1, 18, 20, 22, and 23 have been amended to specify that the claimed methods are computer-implemented methods. Claim 1 has been amended to clarify that selected atoms of the molecules are assigned positions in the one-dimensional representations. Claim 22 has similarly been amended to clarify that at least some atoms of the molecules are assigned positions in the linear representations. Claim 35 has been amended to clarify that the linear representations comprise a set of atoms and associated linear positions in the linear representation. The amendments not related to computer implementation make explicit what was previously implied by the claims. Accordingly, these amendments are not believed to narrow the scope of the claims. Claims 1-35 remain pending in the application. The Applicants have carefully considered all of the Examiner's rejections but respectfully submit that the claims are allowable for at least the following reasons.

Double Patenting

The Examiner provisionally rejected Claims 1-35 under 35 U.S.C. § 101 for statutory double patenting relative to co-pending Application No. 09/770,510. The Applicants believe it is appropriate to wait until either the claims in the instant application or the co-pending application are otherwise in condition for allowance to address the double-patenting rejections. *See* M.P.E.P. § 804(I)(B) ("The 'provisional' double patenting rejection should continue to be made by the examiner in each application...unless that 'provisional' double patenting rejection is the only rejection remaining in one of the applications. If the 'provisional' double patenting rejection in one application is the only rejection remaining in that application, the examiner should then withdraw that rejection and permit the application to issue").

Rejections under § 101 – Subject Matter

The Examiner rejected Claims 1-11 and 18-29 under 35 U.S.C. § 101 as being directed to non-statutory subject matter. The Examiner helpfully indicated that the rejections could be overcome by specifying that the claimed methods were to be computer implemented. The Applicants have amended independent Claims 1, 18, 20, 22, and 23 accordingly. Thus, the

Applicants respectfully submit that Claims 1-11 and 18-20 are now directed to statutory subject matter.

Rejections under § 102

The Examiner rejected Claims 1-35 under 35 U.S.C. § 102(e) as being anticipated by U.S. Patent No. 6,453,246 (Agrafiotis et al.). Agrafiotis discloses representing objects (e.g., molecules) as points in a multi-dimensional space. *E.g.,* abstract ("points in a multi-dimensional space"); col. 5, lines 49-50 ("objects...represent[ed] in a multi-dimensional space"); col. 11, lines 65-66 ("objects...represented as vectors in multi-variate property space"); col. 19, lines 9-10 ("The display map has a point for each of the selected compounds."). As such, each object representation in Agrafiotis will consist of a single point characterized by a plurality of coordinates. Comparisons between multiple objects are evaluated by the distance in the multi-dimensional space between the points associated with each object. *See e.g.,* col. 5, lines 29-33. In contrast, molecules in the present invention are represented by positioning atoms of the molecules in one-dimensional representations. Agrafiotis does not disclose representing individual atoms in a one-dimensional representation of a molecule.

Specifically, Claim 1 requires one-dimensional representations of molecules where selected atoms of the molecules are assigned positions in the representations. Agrafiotis does not disclose representations of a molecule where individual atoms are positioned in the representation. Instead, whole molecules are represented by single points in a multi-dimensional property space without reference to individual atoms in the molecule. Thus, Claim 1 and dependent Claims 2-11 are not anticipated by Agrafiotis.

Claims 12, 23, and 30 require associating or assigning a scalar value (e.g., a one-dimensional coordinate) to individual atoms in a molecule. Agrafiotis also does not disclose assigning coordinates to individual atoms within a molecule but rather assigns coordinates to the molecule as a whole. *E.g.,* col. 19, lines 9-10 ("The display map has a point for each of the selected compounds."). Accordingly, Claims 12, 23, and 30 and dependent Claims 13-17, 24-29, and 31-34 are not anticipated by Agrafiotis.

Claims 18 and 20 require assigning to atoms in a molecule a position (e.g., a coordinate) along a line (e.g., a one-dimensional representation). As discussed above, Agrafiotis does not disclose assigning positions to individual atoms within a molecule. Accordingly Claims 18 and 20 and dependent Claims 19 and 21 are not anticipated by Agrafiotis.

Claim 22 requires deriving linear representations of molecules where at least some of the atoms in the molecules are assigned positions in the linear representation. As already noted, Agrafiotis does not disclose assigning individual atoms in a molecule to positions in a linear representation. Instead, whole molecules are represented by a single point in a multi-dimensional property space without reference to individual atoms in the molecule. Thus, Claim 22 is not anticipated by Agrafiotis.

Claims 35 requires retrieving linear representations of molecules where the representations comprise a set of atoms and associated linear positions in the linear representation. Agrafiotis does not disclose representing linear positions of individual atoms in a molecule in a linear representation. Instead, whole molecules are represented by a single point in a multi-dimensional space. Accordingly, Claim 35 is not anticipated by Agrafiotis.

CONCLUSION

By the foregoing amendments and remarks, the Applicants respectfully submit that they have overcome the Examiner's rejections and request a timely issuance of a Notice of Allowance.

Please charge any additional fees, including any fees for additional extension of time, or credit overpayment to Deposit Account No. 11-1410.

Respectfully submitted,

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